

Tetrachlorophthalic acid
632-58-6 | DTXSID6060896

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 215 °C

Global applicability domain: Inside

Local applicability domain index: 3.96e-01

Confidence level: 5.35e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Benzenedicarboxylic acid,
2,5-dichloro-

Measured: 306

Predicted: 295

Image not found

Chlorendic acid

Measured: 209

Predicted: 196

Image not found

Benzoic acid, 4-hydroxy-3,5-
diiodo-

Measured: 237

Predicted: 235

Image not found

lophenoxic acid

Measured: 147

Predicted: 171